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TITLE COHERENCE AND CHAOS IN CONDENSED MATTER

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## Coherence and Chaos in Condensed Matter

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### I. Nonlinearity in Condensed Matter -- An Overview

In the last decade, *paradigms* of nonlinear science have become firmly established in experimental and theoretical approaches to condensed matter physics [1,2] -- as well as, many other disciplines [3]. Most importantly, "nonlinear science" requires an interdisciplinary and multifaceted approach -- analysis, computation and experiment. Often the approach involves a new look at old problems, e.g.

- the synergistic use of computers.
- the widespread introduction of concepts such as "solitons," "integrable systems," "topology," "chaotic dynamical systems," "pattern selection and function," "nonlinear mode-reduction" and "collective coordinates."
- the importance of "competing interactions" for inhomogeneity in space-time.

There are important *complementary* ideas such as: (i) *order* (e.g. solitons) arising from nonlinearity in *many*-particle systems and partial differential equations [4]; and (ii) temporal *disorder* (e.g. chaos) resulting from nonlinearity even in *few*-particle systems [5]. Combining such order and chaos is an important challenge to modern theory [6].

The basic notions of "solitons" will be introduced here for integrable systems in *one* space dimension [4]:

*Sine-Gordon* equation

$$\varphi_{xx} - \varphi_{tt} = \sin \varphi$$

*Cubic Nonlinear Schrödinger* equation

$$\psi_{xx} + i\psi_t \pm k|\psi|^2\psi = 0$$

*Toda lattice* equation

$$q_{tt}^{(n)} = e^{q^{(n-1)} - q^{(n)}} - e^{q^{(n)} - q^{(n+1)}} .$$

The practical generalization of solitons to finite energy, long-lived structures is illustrated below with topological solitons, clusters in the vicinity of a structural phase transition [7], and vortex configurations in 2-dimensional easy-plane spin systems (section III). It is emphasized that "solitons" span both disciplines and physical scales, and are often "generic" in that they are labelled by certain key *physical* ingredients rather than specific contexts -- e.g. periodic potentials leading to the SG class of equation.

Turning to topical condensed matter/statistical physics contexts, these are *very* numerous. It is therefore more relevant to appreciate certain general themes which have to be faced by each new application:

1. Soliton types in 1-dimension for scalar fields are of 3 types -- "kinks," "pulses," and "breathers" [4].
2. Strict solitons (solutions of integrable equations) play a *unifying* role for most (perhaps all) exactly solvable systems in many-body, field theory and statistical physics -- in quantum 1-dimension or classical 2-dimension (or 1-space and 1-time). Mappings between quantum solitons, Bethe Ansatz solutions, Baxter solutions, Kac-Moody algebras, etc, are examples [8].
3. Strict solitons are rarely (if ever) of *practical* concern, although they may in some circumstances be good starting points for *perturbation* techniques. Observation of solitons and their physical characteristics become context and application *specific* because of *perturbations* and *fluctuations* with respect to "bare" solitons. Important examples include: impurities, external fields; damping; lattice discreteness; dimensionality; thermal, quantum or critical fluctuations (important for statistical mechanics, transport, nucleation, quantum tunneling, etc.). A good example is provided by modeling of "poling" in piezoelectrics [9].
4. Competitions for ground states and excitations are especially pronounced in the presence of *nonlinearity*, *disorder*, and *low-dimensionality*.
5. Intrinsic inhomogeneous structure ("defects") can often be classified (if they are topological) by, e.g., homotopy theory -- for instance in liquid cristals, $^3$He, crystal defects. This is important because of their relevance to transport and relaxation [10].
6. Intrinsically nonlinear defects play an important role in phase transitions of many kinds -- first order (droplet nucleation), continuous (cluster dynamics), topological, commensurate-incommensurate, multiphase equilibra, "universal" critical short-range-order, etc. Structural phase transitions and incommensurate structures are discussed briefly below.
7. Low-dimensional magnets are good examples of soliton contexts. Quasi-1-D systems ($CsNiF_3$, TMMC, $CsCoCl_3$, ..) have been especially tractable and didactic examples. Quasi-2-D materials ($K_2CuF_4$, $RbCrCl_4$, graphite intercalates...) are increasingly studied in the context of vortices, domains, discommensurations, and most recently high-temperature superconductors. Low-D magnets are considered in section 3.
8. Low-dimensional organic and organo-metallic materials are also contexts where solitons and nonlinear effects more generally are prevalent [11]. These include phenomena such as: broken symmetry ground states (charge density, spin density, superconducting, bond order, etc); competitions (leading to inhomogeneous ground states); nonlinear excitations (especially *self-trapped* states, including polarons, important in physics, chemistry, biophysics). Some of these issues are introduced in section 4.
9. Nonlinear, nonequilibrium phenomena are a growing focus in solid state and material's science, where "complexity" in space and/or time is as important as in areas such as hydrodynamics or plasmas. This field is reviewed in section 2.

*Structural phase transitions* provide good examples in materials science for the evolution of approaches with which to incorporate strongly nonlinear effects. During the period 1970 - 1980 radical changes took place both experimentally and theoretically introducing ideas of incomplete soft modes, central peaks and intrinsic clusters in displacive structural phase transition materials. A one dimensional model (the "$\varphi$-four" or "double well" Hamiltonian) illustrates this [7]:

$$H[U] = \sum_i \frac{1}{2} m \left(\frac{du_i}{dt}\right)^2 + \frac{1}{2} A u_i^2 + \frac{1}{4} B u_i^4 + C(u_{i+1} - u_i)^2 .$$

Here, we consider a unaxial ferrodistortive (spring constant $C > 0$) system with particles of mass m and displacement $u_i$ (from local equilibrium) moving in one-site doubly-degenerate wells ($A < 0$, $B > 0$). In the so-called "displacive" regime ($C \gtrsim |A|$) a continuum approximation is valid leading to the $\varphi$-four equation describing the lattice dynamics:

$$m u_{tt} - 2\, C a^2 u_{xx} - |A| u + B u^3 = 0,$$

where a is the lattice constant.

This equation has low-amplitude and high-amplitude "phonons" as solution (limits of elliptic travelling waves). In addition it supports kinks (domain walls), solitons and long-lived coherent breather-solitons. Attempts to linearize the equations of motion (by "self-consistent" or "renormalized" phonon approximations) suppress the nonlinearity: they can capture the best *harmonic* approximations of high- and low-temperature phonons and suggest that there is a transition between those at a "soft" mode temperature $T_0$. The inclusion of fully nonlinear kink solitons renders this softening incomplete and shows that it is accompanied by a "central peak" (i.e. scattering intensity around frequency $\omega = 0$). This is illustrated in Fig. 1.

The central peak narrows and grows as $T \to 0$ corresponding to the density of kinks $\to 0$ and complete long-range order appearing. In dimensions greater than unity a phase transition to long range order occurs at a *finite* temperature $T_c$ even for short-range interactions. Again, however, $T_c < T_0$. We illustrate this situation with results [7] on *weakly-coupled* chains of double-well-potential particles, representative of anisotropic ferroelectrics (e.g. $CsD_2PO_4$), Peierls-distorted chains (e.g. KCP), etc. Here a *mixed* phase of displacive behavior on-chain but order-disorder ($C \gg |A|$) between chains occurs, and $T_c \ll T_0$ so that the 1-dimensional short-range-order regime is enhanced and 2-dimensional crossover occurs only close to $T_c$. The general scenario of order-disorder-displacive crossover in double-well systems of general dimension can be presented as in Fig. 2.

*Commensurate-incommensurate* phase transitions are now widely encountered (in theory *and* experiment) in a large range of physical circumstances [12]. The key physical ingredient is the occurrence of *competing interactions*. We argue in section 2 that these are also a central concept for dynamical systems (showing "complexity" in space time) quite generally. Here we describe purely static contexts of *competing spatial* scales. The physical variable sensitive to the competition may be displacement, mass, spin, charge-density, phase, rotation, pitch, etc. The physical contexts are equally diverse -- epitaxy, charge-density-waves, ANNNI magnets, ferroelectrics, crystal faceting, etc.

The competitions for length scale characteristically result in spatially *inhomogeneous* thermodynamic phases. The *appearance* of homogenous commensurate regions in space, separated by inhomogenous incommensurate segments ("discommensurations") is typical. The density of discommensurations then $\to 0$, as the incommensurate-commensurate phase transition is approached, eventually leaving a fully locked (homogeneous commensurate) pattern. This scenario is illustrated by a simple 1-dimensional surface epitaxy model, after the style of Frenkel-Kontorova or Franck-van der Merwe, with Hamiltonian [12]:

$$H = \sum_n \left[\frac{1}{2} m \left(\frac{dx_n}{dt}\right)^2 + V\left(1 - \cos\left(\frac{2\pi x_n}{b}\right)\right) + \frac{1}{2} C(x_{n+1} - x_n - a)^2\right] .$$

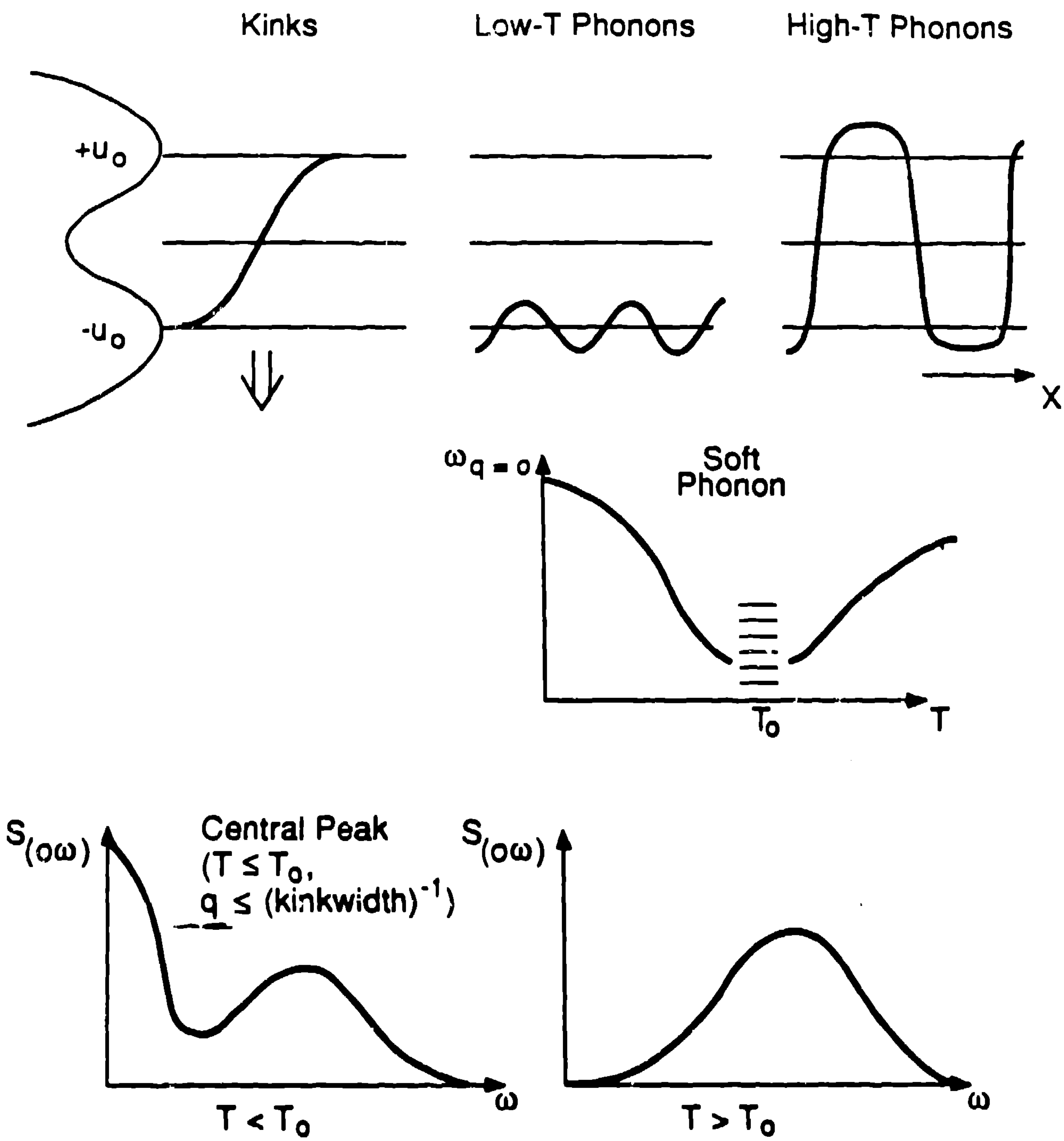


Figure 1. Central peak formation and anharmonic phonon softening in a 1-D $\phi^4$ model (see text).

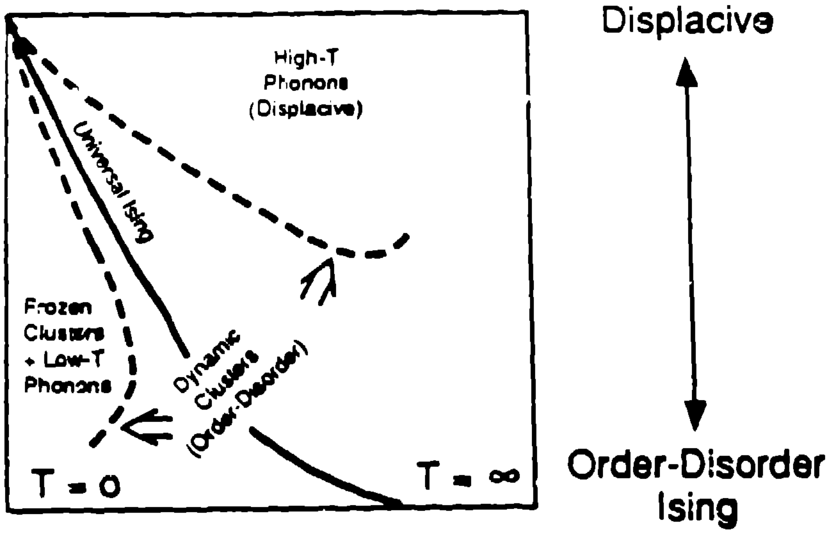


Figure 2. Cluster and anharmonic phonon regimes in displacive-order disorder $\phi^4$ models.

Here, $x_n$ is the displacement of the n-th particle (mass m) of the epitaxial layer moving in a periodic substrate potential of strength V. There are *two* characteristic length scales: (a) the natural epitaxial layer lattice periodicity, a, set by the harmonic inter-particle spring C: and (b) the substrate periodicity, b. In general a and b can be incommensurate (irrationally related). A discommensuration superlattice then takes the schematic form shown in Fig. 3 where $\theta$ is a deviation relative to a particular superlattice order: $X_n = nbP + b\theta_n/2\pi$, with $Qa = Pb$, Q and P irrationally related integers.

Important generalisations of the above discommensuration model include: effects of a discrete lattice [13] (including "chaotic" discommensuration pinning, locked phases); interactions between discommensuration lines (leading to structural transitions and melting of discommensuration superlattices) [12]; dynamics in the presence of competing interactions (phason modes, hysteresis and metastability); and generalisations to include *multiple* competing length scales and *non-convex* interparticle springs [14]. These last ingredients are becoming of direct concern in *materials science* applications of competing interactions such as martensite materials, polytypes, polymers, grain-boundary structure.

## II. Coherence and Chaos in Spatially Extended Condensed Matter Systems

The focus of dynamical systems research has now moved strongly towards *spatially extended* systems [6,8]. This naturally brings together ideas of *pattern formation* and *chaos* -- varying degrees of "complexity" may occur in space or time or both, as is experienced in many areas of the natural sciences, from astrophysics to biology. Our particular concern is with examples from condensed matter physics which has some

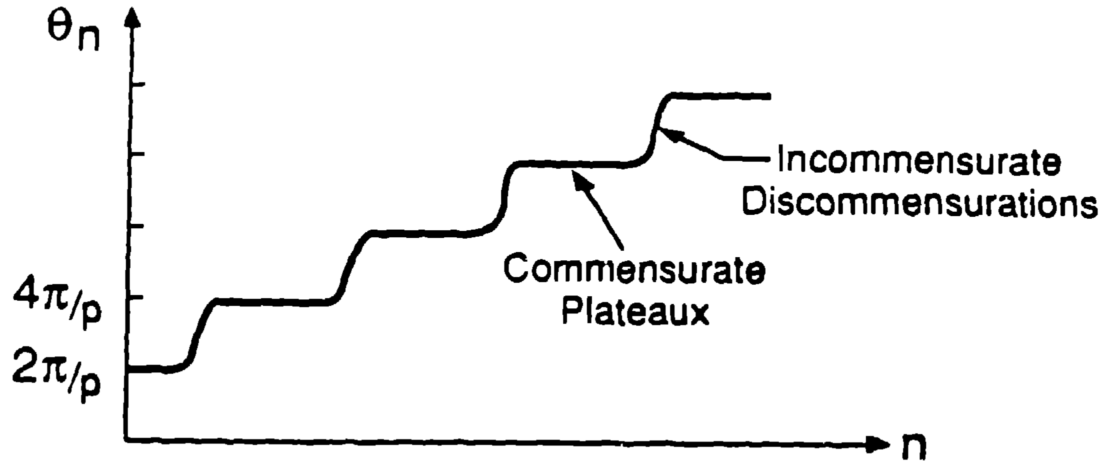


Figure 3. A discommensuration array in the Frenkel-Kontorova model: see text.

special advantages. In particular, these systems are frequently "bench-top" size and concern materials and experiments which are well controlled. In addition, control of geometry and dimensionality are novel, and questions of space-time complexity are of direct practical interest for device performance, e.g. in Josephson transmission lines.

These considerations have lead us to study [6,8,15] *chaos* and *coherence* (usually in time and space, respectively, but not exclusively) in a variety of nonlinear partial differential equations modeling specific condensed matter materials and experimental models thereof -- Josephson junctions and lines, pinned charge-density-waves, low-dimensional magnets, oscillating water tanks, etc. We also anticipate a rapid growth in the appreciation of these issues for more traditional materials applications -- the importance of space-time inhomogeneous structures for strength and response is generally recognized but there is a need for much greater unification and dynamical systems approaches to complexity may provide this. [See, e.g., articles in "Competing Interactions and Microstructures," eds. R. LeSar, A. Bishop, R. Heffner (Springer-Verlag 1988).]

There a three separate (but merging) types of problems so far addressed in condensed matter contexts:

1. *Structural disorder* and inhomogeneity in (classical) static Hamiltonian systems with *competing* (incommensurate) interactions or periods. Such competitions occur in a large variety of solid state materials exhibiting commensurate-incommensurate phase transitions [12]. They are responsible for regular or irregular arrays of "discommensurations" as ground states, for "devil's staircases" of locking transitions between commensurate uniform states, hysteretic dynamics, etc. [12,13]. Studies of multiple competing lengths [14] and of large-scale *dynamics* are important and in their infancy.

2. Space- *and* time-dependent (classical) systems corresponding to nonlinear partial differential equations or coupled systems of nonlinear ordinary differential equations arise naturally as models of condensed matter. Driven, damped equations such as the sine-Gordon and nonlinear Schrödinger systems have been particularly well studied in various spatial dimensions and with various boundary conditions. These provide excellent examples of mode excitation, nonlinear saturation, conversion and competition (leading to complexities including temporal chaos). As well as being close models of specific experimental situations, they have the advantage of being integrable in the absence of perturbations. Thus a tractable nonlinear mode basis of strict solitons is available in which to project perturbed flows. References [6,15] describe this scheme in detail for the periodic sine-Gordon ring. Many of the lessons quantified by this "near-integrable" approach extend to far more general situations. Indeed it is increasingly appreciated that there are typical ways that space-time attractors (either chaotic or as routes to chaos) are manifested. In this regard, it is important to appreciate that there are several approaches taken to study extended dynamical systems -- in addition to specific (classes of) p.d.e.'s, cellular automata [16] (various discretizations of p.d.e.'s) and coupled "lattices" of low-dimensional maps [17] are also widely investigated. Most importantly, synergetic *mappings* are gradually becoming apparent within and between these seemingly different approaches to space-time attractors. Furthermore, there are additional mappings to higher dimensional effective Hamiltonians (with time being replaced by an auxilliary space). These effective Hamiltonians exhibit *competing interactions* [18]. Thus, the conceptual framework for "inhomogeneous" space-time attractors is the *same* as for purely spatial chaos in (1). Competing interactions are the key feature and spatial discommensurations become analogous to space-time intermittency. Orderly temporal behavior is usually accompanied by (higher symmetry) spatial pattern formation and irregular temporal behavior by a breaking of that spatial symmetry. However, "chaos" is usually low-dimensional because it is characterized by a small number of highly coherent (~soliton) structures moving irregularly in a sea of extended ("radiation") modes (which may be active, slaved or heat-bath in character). The "solitons" become locked in phase and amplitude when a higher symmetry spatial pattern stabilizes. A typical example is shown in Fig. 4, where a period sine-Gordon ring is being driven by a homogeneous ac-field with homogeneous damping.
   Since the number of p.d.e. studies of chaos continues to grow rapidly, we merely include here a representative guide to the literature:
   Recent studies include: sine-Gordon-like systems with periodic [6,8,19] Neumann [8] or absorbing [21] boundary conditions, including 2-D [22] cases and discrete generalizations [8]; nonlinear Schrödinger equations [8], including models of plasmas [23], bistable optical ring oscillators [8], coupled acoustic oscillators and surface waves, and complex generalizations such as Landau-Ginzburg [8,24], the Korteweg-de Vries equation, Toda lattice and generalizations [25]; classical spin chains; Kuromoto-Sivashinsky and similar equations for interface dynamics [6]; and finite pole or theta-function representations [6,8]. Finally, we reemphasize the closely related types of space-time complexity observed in studies of coupled map lattices [17] and of cellular automata [16].
   An excellent cross-section of these studies, together with articles describing physical systems being investigated experimentally, is contained in the conference proceedings of Ref. [6].
3. "Quantum Chaos" is described in detail in the lectures of GUTZWILLER. The notion of studying Hamiltonian and dissipative quantum systems which have well-defined classical limits is itself well-defined and of clear experimental

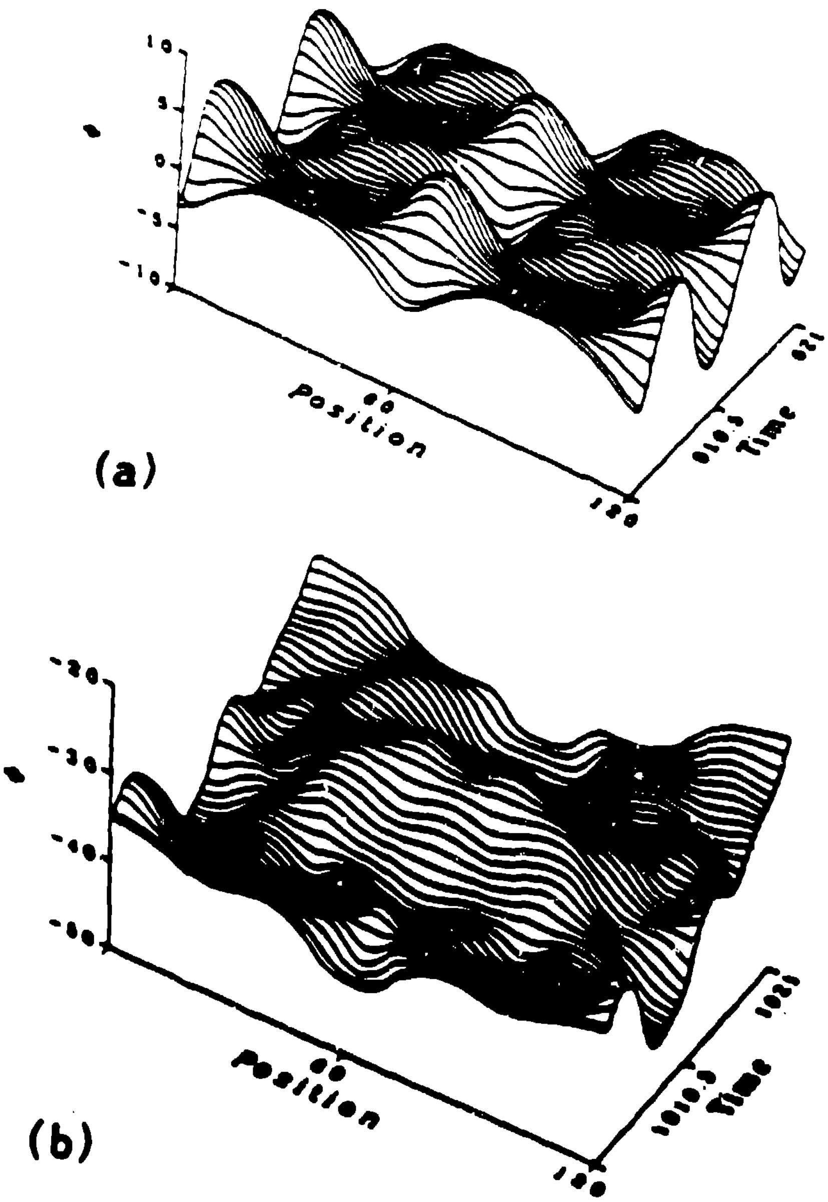


Figure 4. Space-time evolution for a periodic Sine-Gordon chain with damping $\epsilon\phi_t$ ($\epsilon$ = 0.2) and homogeneous ac-driving $\Gamma$ sin($\omega_d t$) ($\omega_d$ = 0.6). Evolution is shown for approximately two periods of the driver with: (a) $\Gamma$ = 0.8, which results in periodic time evolution of a spatially period-1/2 pattern; and (b) $\Gamma$ = 1.0, which results in chaotic kink-antikink motions, nearly repeating each driving period. The important dynamics here is that of kink-antikink collisions mediated by certain phonons, resulting in a *slow* diffusion of the center of mass as in dislocation slippage in metals (note the ranges of $\langle\phi\rangle$ in cases (a) and (b)).

relevance. Furthermore, combining these problems with dynamical systems approaches, since they have in recent years become more widely recognized and appreciated, is tempting. Several models motivated by solid state or statistical physics are interesting in this regard. In particular *spin* problems have the advantage of a finite manifold which makes computation of energy levels and wavefunctions very controlled numerically. We have focused on two systems in detail: (i) a triangle of *3* Heisenberg spins coupled antiferromagnetically [26];

$$H = J \sum_{1}^{3} (\vec{S}_i \vec{S}_{i+1} + \sigma S_i^z S_{i+1}^z) ;$$

and (ii) a *single* Heisenberg spin with easy-plane anisotropy and a periodically pulsed magnetic field applied in the easy-plane [27].

$$H = A(S_z)^2 - \mu B S_x \sum \delta(t - 2\pi n) .$$

Both examples have the crucial advantages of being able to readily vary the "quantumness" (h~ $S^{-1}$) and the degree of non-integrability (in the first case by controlling spin space symmetry $\sigma$ and in the second via the magnetic field strength B). The tunability of these parameters has lead us to identify new scaling and self-similarity properties both in the distribution of energy levels and in the associated wave functions. Details are contained in Refs. [26,27]. Evidently, a whole field of new studies are available here, extending these kind of studies to many-particle systems (e.g. perturbing around exact soliton-bearing or Bethe Ansatz models) and including dissipation - - the combination of these two ingredients leads immediately to questions of macroscopic quantum tunneling [28].

## III. Nonlinearity and Magnetism

Magnets have provided examples of strong nonlinearity for many decades - - they provide numerous systems where we (at least believe we) have good microscopic descriptions. Magnetic domain walls are as well studied as dislocations, and their structure and dynamics are of immediate importance in coercive magnetic devices - - including bubble devices studied until recently for their information storage potential. Domain wall response to magnetic fields leaves much to be understood (except at low fields where "particle" like dynamics is often adequate) [29], and may provide good examples of longitudinal or transverse instabilities on propagation interfaces [30].

In the more recent developments of soliton literature, magnets have been important for several reasons:

1) They provide numerous examples of exactly integrable solvable equations - - both classical (in 1 + 1 and 2 + 0 dimensions) and quantum (1-dimensional). Indeed the original Bethe problem (a S - $\frac{1}{2}$ isotropic Heisenberg ferromagnetic chain and the Onsager 2-dimensional Ising model can be mapped directly into soliton systems). Many generalizations (classical and quantum mechanical) have been explored in the last decade [31,32], but a simple example, the *classical isotropic* continuum Heisenberg model in one space dimension, will serve to illustrate the mathematical beauty of these systems:

Here [32] the Hamiltonian for the spin field $\vec{S}(x,t)$ takes the form

$$H\{\vec{S}\} = \frac{1}{2}\int dx [\frac{\partial \vec{S}}{\partial x}]^2$$

and the equation of motion is

$$\frac{\partial \vec{S}}{\partial t} = \vec{S}\ \frac{\partial^2 \vec{S}}{\partial x^2} .$$

Natural canonical variables are $p = S^z = \cos\theta$ and q, where $S^x = (1 - p^2)^{\frac{1}{2}} \cos q$ (q $= \phi$). In these variables it is evident that the system is nonlinear and that there is no simple decomposition into kinetic and potential energy:

$$H(\{p\},\{g\}) = \int dx\ \{\frac{1}{1-p^2}\ (\frac{dp}{dx})^2 + (1-p^2)(\frac{dg}{dx})^2\} .$$

The exact integrability of this system follows from the identification of a "Lax-pair" (L,M) representation for the spin variables [32]:

$$S = \vec{S} \times \vec{\sigma} = \begin{pmatrix} S^z & S^- \\ S^+ & -S^z \end{pmatrix}$$

$$\frac{dS}{dt} = \frac{1}{2i}\ [S, \frac{d^2S}{dx^2}]$$

$$L = S\frac{d}{dx}\ \ ;\ \ M = 2S\frac{d^2}{dx^2} + \frac{dS}{dx}\frac{d}{dx}$$

$$\frac{dL}{dt} = i\ [L, M] .$$

The operators L and M are linear and non-selfadjoint, and operate in a space of dependent $2 \times 2$ matrices. It is straighford to include a field term $\vec{H}_0 \times \vec{S}$ by a gauge transformation. Strictly speaking, "decaying" boundary conditions are required, viz. $\lim_{|x|\to\infty} S(x,t) = \sigma^z$. A similar structure for periodic boundary conditions is however possible.

Following the procedures of inverse scattering theory [4], an associated *linear* eigenvalue problem can be identified,

$$iL\psi = \lambda\psi$$

$$i\frac{d\psi}{dt} = M\psi ,$$

where the spectrum $\{\lambda\}$ has the remarkable property of being time invariant. The spectrum comprises both discrete ($\leftrightarrow$ "soliton") and continuum ($\leftrightarrow$ "magnon") components. Asymptotic scattering data can be evolved according to the above prescription and the inverse step (the Gel'fand-Levitan-Marchenko integral equation) gives S(x,t) from the evolved data. In this way, arbitrary initial data can be decomposed into "nonlinear normal modes" and followed in time. Further, it is possible to identify new *canonical* variables, $P(\lambda)$, $Q(\lambda)$, from the scattering data, which are natural action-angle variables:

$$\{Q(\lambda), Q(\lambda')\} = \{P(\lambda) P(\lambda')\} = 0$$
$$\{P(\lambda), Q(\lambda')\} = \delta(\lambda - \lambda')$$
$$P(\lambda) \geq 0 \ ; -2\pi \leq Q(\lambda) \leq 0$$
$$\{Q_n, Q_m\} = \{P_n, P_m = 0$$
$$\{P_n, Q_m\} = \delta_{nm} : Re(P_n) > 0 \quad .$$

This action-angle set is extremely conveniant as a starting point to discuss statistical mechanics or quantization, as can be seen by the "separable" form that conserved quantities take. For example, the Hamiltonian becomes

$$H = 4 \int_{-\infty}^{\infty} d\lambda \ P(\lambda) \ \lambda^2 + 4 \sum_{n=1}^{V} (\frac{1}{Pn} + \frac{1}{\bar{P}n}) \ ,$$

where $\bar{P}$ is complex conjugate. The first term has the form of continuum (magnon) states: defining energy $\varepsilon(\lambda) = 4\lambda^2$ and momentum $\pi(\lambda) = 2\lambda$, we have $\varepsilon(\lambda) = \pi^2(\lambda)$. The second term is the soliton contribution (in real space these are pulse structures [33]): defining $P_n = A_n \, e^{-i\theta/4}$, it is possible to express the energy as $\varepsilon = \frac{16}{|m_n^z|} \sin^2(\pi/4)$, where $\pi_n$ and $m_n^z$ are the linear- and z-component of angular-momentum, respectively.

As in section I, we emphasize that the apparent separability of H is somewhat deceptive. This is a nonlinear system and modes *do* interact, but in such integrable models the interaction is purely via reciprocal phase (space)-shifts. Nevertheless, these phase shifts are responsible for changes in density-of-states and these restrictions on available phase space are of crucial importance, precisely as in Bethe Ansatz quantum schemes.

2) Many *real* low-dimensional magnetic materials (chain and layer-like) exist [34,35]. They can be well-synthesized and controlled measurements of thermodynamic and scattering properties can be made. For this reason, linear theories of magnets have long found good experimental test-beds [34], and this has naturally also become true of soliton theories. Because the material basis is sound, low-dimensional magnets have also served to emphasize an important salutory lesson for solitons in real materials: the soliton paradigm is intended to be a guide to an improved *starting point* for theory and experimental design/interpretation. It is not a universal panacea and each context demands attention to specific important perturbations. Thus, in the case of easy-plane ferromagnetic chains (e.g. $CsNiF_3$), it is rather clear that a sine-Gordon-like system will govern in-plane dynamics in the presence of an in-plane magnetic field. If we take the Hamiltonian [36],

$$H = -J \sum_n \vec{S}_n \, \vec{S}_{n+1} + A \sum_n (S_n^z)^2 - g\mu_B \, B^x \sum_n S_n^x$$

with dynamics

$$\vec{S}_t = \{H, \vec{S}\}$$

and *linearize* in the out-of-plane spin angle $\theta$, then we find immediately that

$$\phi_{tt} = c_0^2 \phi_{zz} - \omega_0^2 \sin \phi$$

$$2AS\theta = \phi_{tt} \ .$$

where $\phi$ is the in-plane spin angle, $c_0^2 = 2AJa^2S^2$, $\omega_0^2 = 2Ag\mu_B DS$, a is a lattice constant, and we have assumed that a continuum ($z$) description is valid. This sine-Gordon approximation is very well documented and is indeed a good playground for testing sine-Gordon statistical mechanics -- experimental measurements of specific heat and inelastic neutron scattering have been especially careful [35]. However, while qualitative agreement with sine-Gordon theory was initially appealing, it has taken several years to appreciate that subtler effects play very important roles too. For example, central peaks in dynamic structure factors may have kink soliton contributions but (depending on which correlation is measured), essentially linear multimagnon and bound multimagnon ("breather") contributions are also major components. Again, linearizing in $\theta$ is a very poor approximation in *classical* dynamics -- nonlinear out-of-plane effects produce binding and even repulsion during kink-antikink collision rather than sine-Gordon transmission [37]. This appears to be somewhat compensated by *quantum* effects which may act to inhibit motions out of a zero-point plane. However, the combined effects of quantization and nonlinear out-of-plane fluctuations have even now not been fully resolved -- especially for dynamics. A very similar situation applies to other easy-plane ferromagnets (e.g. CHAB, where quantum Monte Carlo even questions the validity of the assumed Hamiltonian [38]) and to easy-plane antiferromagnets (e.g. TMMC) [39]. Figure 5 illustrated "breather" formation in the case of a kink-antikink collision in a classical antiferromagnetic model.

*Two-dimensional* magnets are an equally rich hunting ground for nonlinear excitations. The prospects for studying *dynamics* associated with the Kosterlitz-Thouless transition are beginning to look especially appealing, with controlled inelastic neutron scattering experiments being made on several layered materials [40]. (e.g. $K_2CuF_4$, $Rb_2CrCl_4$, $BaCo_2(AsO_4)_2$) Phenomenological theories, based on ideal gases of vortex excitatiors moving in a screening environment of bound vortex-antivortex pairs [41], compare well with numerical simulations and have many of the qualitative features seen experimentally. Other excellent two-dimensional magnets include graphite intercalated with magnetic ions (e.g. $CoCl_2$) and surface layers.

Finally, we reemphasize the prospects for low-dimensional magnets as experimental environments in which to study coherence and chaos (Section II); and note the relations to stoichiometric Cu-O layered materials which exhibit high-temperature superconductivity under doping.

## IV. Solitons and Conducting Polymers

Conjugated polymers such as suitably synthesized polyacetylene have emerged as prototypes of an intriguing class of "synthetic metals" -- synthetic materials with metallic properties (in this case, nearmetallic levels of conductivity upon sufficient doping). Not surprisingly, the vast body of research on this class of matrials is driven by the needs for new syntheses and the potential for applications (for example in batteries or nonlinear optics) [11]. However, theoretical modeling of the (by now) many examples of conducting polymers has lead to a rich interdisciplinary story in its own right. First, the field has provided a basis for interdisciplinary collaborations between field theorists, solid state theorists and quantum chemists. Second, soliton ideas (although at first sight quite straightforward -- see below) have found exotic variations -- including connections to exactly solvable field theories and to fractionally charged species. Indeed, all the "simple" solitons mentioned in Section I (kinks, pulses and breathers) have found a home in polyacetylene models. Third, these materials are important examples of the increasingly urgent search for novel materials and they emphasize our need to explore *mesoscale* materials, for which current elec-

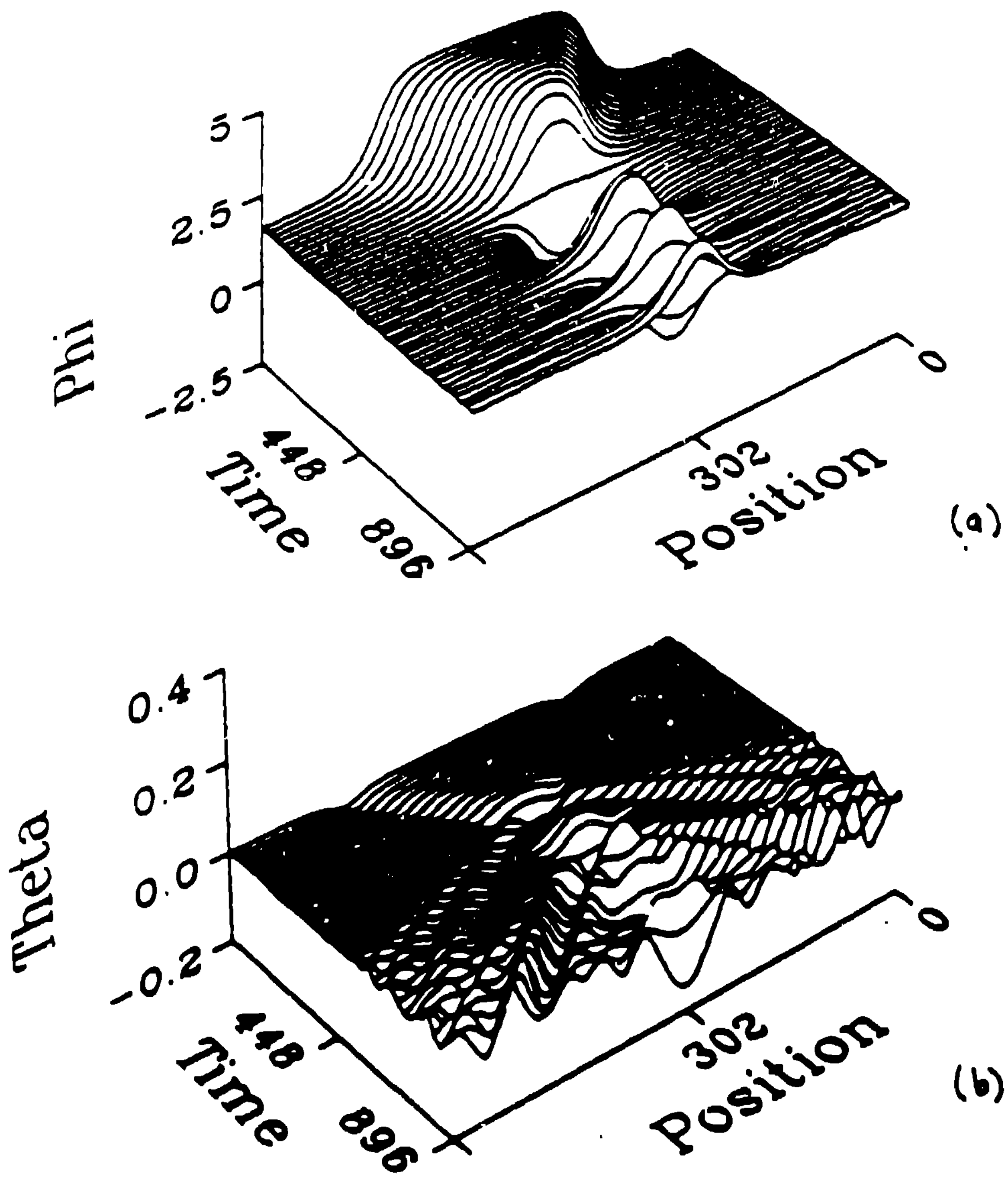


Figure 5. Breather formation following soliton-antisoliton collision in an easy-plane ferromagnet with in-plane magnetic field.

tronic structure theory is frequently poorly prepared. In these cases we are confronted with material sizes which are intermediate between small polyenes (the realm of quantum chemistry) and macroscopic semiconductors (the realm of solid state). Schemes applicable in the two limits have to be rethought in the mesoscale regime. Fourth, low-dimensionality and disorder introduce *competitions* for ground states and excitations. Conducting polymers represent a member of a growing class of such environments, where *collective* ground states are in sensitive competitions -- spin-and-charge-density, bond-order, superconducting ferroelectric, etc. Ultimately, conducting polymers may be best thought of as semiconductors but with disorder on many length scales and with extreme anisotropies. In this regard also they correspond to a *new* class of materials for experimentalists and theorists. The primary charge carriers are *probably* "polaronic" in character but the influences of disorder, anisotropy, electron-electron interactions, interchain coupling, etc., have yet to be fully understood.

For a review of the current state of the evolving art, the reader is referred to [11,42,43]. For the present purposes, it is sufficient to briefly indicate how models of isolated polyacetylene chains have provided natural examples of *kinks* (domain walls), *pulses* (polarons) and *breathers* (anharmonic phonon wave-packets) -- in ideal polyacetylene it is now believed that *inter*chain coupling is very important. To this end we restrict ourselves to the simplest model of Su-Schrieffer-Heeger for trans-polyacetylene with purely electron-phonon coupling [14]:

$$H = -\sum_{n,s}(t_{n+1,n}\, C^{+}_{n+1,s} C_{n,s} + h.c.) + \frac{K}{2}\sum_{n}(U_{n+1} - U_n)^2 + \frac{1}{2} M \sum_{n} \dot{U}_n^{\,2} .$$

Here M is the mass of C-H unit, $C^{+}_{n}$ is a creation operator for a $\pi$-electron at the n-th site, $U_n$ is the displacement of the n-th C-H unit from an equal bond length configuration, and K is the spring constant between neighboring C-H units. The transfer matrix element incorporates electron-phonon coupling in the form

$$t_{n+1,n} = t_0 - \alpha(U_{n+1} - U_n) ,$$

where $\alpha$ is the coupling constant. Direct studies of the adiabatic ground state show that the equal bond length configuration is unstable towards uniform *dimerization* $U_n = \pm\, (-1)^n\, U_0 = \pm\, \tilde{U}_0$. This is referred to as a Peierls dimerization since the $\pi$-electron band is initially half-filled. This "spontaneous broken symmetry ground state" is accompanied by a gap appearing at the Fermi level. Both the size of the dimerization and of the electronic gap are determined by $\alpha$.

In the limit of weak coupling, a continuum approximation is valid in terms of the staggered order parameter $\tilde{U}(y)$ and an electronic spectrum linearized about $\pm\, k_F$. Then [45,46]

$$H = \sum_{s} \int dy \,\{ \frac{\omega_Q^2}{2g^2}\, \Delta^2(y) - iV_F U(y)\, \frac{\partial U(y)}{\partial y} + iV_F V(y)\, \frac{\partial V(y)}{\partial y} + \Delta(y)[U^*(y)V(y) + V^*(y)u(y)]\} ,$$

with $\Delta(y)$ and $g(M/a)^{\frac{1}{2}}\, \tilde{U}(y), g = 4\alpha(a/M)^{\frac{1}{2}}, \omega_Q^2 = 4K/M$, and $(U(y), V(y))$ the spin or electronic field. Variation of H with respect to U, V and $\Delta$ yields the following set of equations to be solved self-consistently

$$E_n\, U_n(y) = -iV_F\, \frac{\partial U_n(y)}{\partial y} + \Delta(y) V_n(y)$$

$$E_n\, V_n(y) = -iV_F \frac{\partial V_n(y)}{\partial y} + \Delta(y) U_n(y)$$

$$\Delta(y) = \frac{-g^2}{\omega_Q^2} \sum_{n,s}{}' \, \{V_n^*(y) U_n(y) + U_u^*(y) V_n(y)\}\ ,$$

where prime indicates summation up to the Fermi level. These equations have the form of a Dirac-like equation in a y-dependent potential $\Delta(y)$ with a subsidiary "gap" condition. Their solutions represent *all* possible *static* adiabatic solutions to the Su-Schrieffer-Heeger model. Remarkably, *all* such solutions can be obtained *exactly* and *constructively* using inverse scattering techniques [46]. Furthermore, this exactly solvable problem is *exactly equivalent* to a popular field theory model, the Gross-Neveu model of quadratically coupled, massless fermions. The most general Gross-Neveu model Lagrangian includes fermions with N "flavors:"

$$L = \sum_{\alpha=1}^{N} \bar{\varphi}^{(\alpha)}(y)\, (i\gamma_\mu \frac{\partial}{\partial y})\, \varphi^{(\alpha)}(y)$$

$$+ \frac{1}{2}\, g_{G.N}^2 \;\; [\sum_{\alpha=1}^{N} \bar{\varphi}^{(\alpha)}(y) \varphi^{(\alpha)}(y)]^2\ .$$

(See Ref. [46] for notation).

The polyacetylene case corresponds to $N = 2$ ($\pm\, k_F$ electrons), but $N = 1$ and 4 have also found solid state analogues [46,47]. In addition new solvable models have been motivated by solid state materials (e.g. ordered A-B alloys and cis-polyacetylene [46,48]) which have lead to new solvable field theories being identified. Finally, the *incommensurate* Peierls model is equivalent to the $N = 2$ *chiral* Gross-Neveu model [46].

The availability of these exactly solvable models is of course important for many benchmark calculations -- for example of optical absorption [49] or polaronic masses. These are especially interesting in field theory because they provide explicit examples of "dynamical mass generation" (the equivalent of the spontaneous dimerization -- i.e., gap formation), and of "negative energy sea anomalies." These anomalies include the exotic notion of "fractionally charged solitons," and are the consequences of phase shifts suffered by the valence band extended electronic states in the presence of soliton defects [49].

We limit ourselves here to a description of the elementary "soliton" excitations supported by the $N = 2$ Gross-Neveu model [46]. In the language of our polyacetylene model these appear as:

(a) ***kinks*** or ***domain walls*** with

$$\Delta_K(y) = \pm \Delta_0\, tanh\, \frac{y - y_0}{\xi_0}\ ,$$

where $\xi_0 = V_F/\Delta_0$, a coherence length ($\sim$5-10 a in polyacetylene). In addition to phase shifting of valence (and conducting) band states, the kink produces another *localized* electronic state exactly at the middle of the electronic energy gap, i.e. at the Ferm level (this a consequence of an exact electron-hole symmetry).

(b) ***polarons and bipolarons*** with:

$$\Delta_P(y) = \Delta_0 - K_0 V_F \; \{tanh \; K_0(y + y_0) - tanh \; K_0(y - y_0)\} \; ,$$

where $2K_0 y_0 = \tanh^{-1}(K_0 V_F/\Delta_0)$. The polaron interpolates between pure dimerization ($\omega_0 \rightarrow \Delta$) and an infinitely separated $K\bar{K}$ pair ($\omega_0 \rightarrow 0$). Since the polaron has the form of a kink-antikink pair, it is not surprising that the associated electronic spectrum contains *two* states localized in the gap, symmetrically distributed about the Fermi level -- at $\pm\,(\Delta_0^2 - K_0^2 V_F^2)^{\frac{1}{2}}$.

The state of charge (and spin) of the above intrinsic defect states is determined by the occupation of the localized gap states. Possible kinks, polarons and bipolarons are illustrated in Fig. 6.

Importantly, while kink and polaron states are possible in trans-polyacetylene, only polarons and bipolarons are allowed in cis-polyacetylene. This distinction occurs because the ***degenerate*** ground states in trans-polyacetylene are available in cis-polyacetylene, where an additional term in the Hamiltonian breaks the degeneracy. This results in a ***confinement*** of kink-antikink pairs so that free kinks are not possible [46]. The situation is easily understood in chemical terms as shown in Fig. 6, where single and double bonds correspond to long and short CH near-neighbor separations.

Since most conducting polymers presently synthesized have fallen into the cis-polyacetylene category (a unique ground state and a metastable second configuration), experimental and theoretical attention has moved strongly toward their identification. Combinations of optical absorption, ESR, doping-induced spectroscopy and photoexcitation studies, now strongly support their presence [11]. While it is likely that they play a major role in transport, a great deal of research remains to elucidate details.

We conclude this section with very brief remarks on ***adiabatic dynamics***, which allows us to introduce the final "soliton" excitation, referred to above, namely a ***breather***. These appear as coherent anharmonic phonon packets with associated oscillatory electronic energy levels. They have been proposed as important features of kink propagation and photoexcitation (across the ground state gap or in the presence of localized gap states due to polarons or extrinsic impurities) [50]. As one example, consider photoexcitation of an electron from the top of the valence band to the bottom of the conduction band within the Su-Schrieffer-Heeger model. As shown in Fig. 7, this initial condition very rapidly (after $\sim 10^{-13}$ sec) evolves into a separating kink and antikink and a localized envelope structure oscillating periodically in time (see Fig. 7(b). The kink and antikink separate at a ***maximum*** velocity where their combined kinetic energy is $\sim 0.2\ \Delta_0$ [50]. The oscillatory mode can be described very accurately in terms of "soliton" (breather) solutions of a nonlinear Schrödinger equation. These have the form [50]

$$\Delta(x,t) = \Delta_0[1 + \delta(x,t)]$$

$$\begin{aligned} \delta(x,t) \;&=\; \epsilon\sqrt{6} sech\,(\epsilon\,\sqrt{12}\,x/\xi_0)\,cos[1 - \frac{1}{2}\epsilon^2)\omega_R\,t] \\ &+ \frac{3}{2}\,\epsilon^2 sech^2\,(\epsilon\sqrt{12}\,x/\xi_0)\{\frac{1}{3}\,cos[2(1 - \frac{1}{2}\epsilon^2)\omega_R\,t] - 1\} \\ &\qquad \omega_R = \omega_0(\lambda)^{\frac{1}{2}} \quad . \end{aligned}$$

and energy

$$E_B = \Delta_0\,\frac{2\sqrt{3}}{\pi}\,\epsilon[1 - \frac{5}{9}\,\epsilon^2 + o(\epsilon^4)]\; ,$$

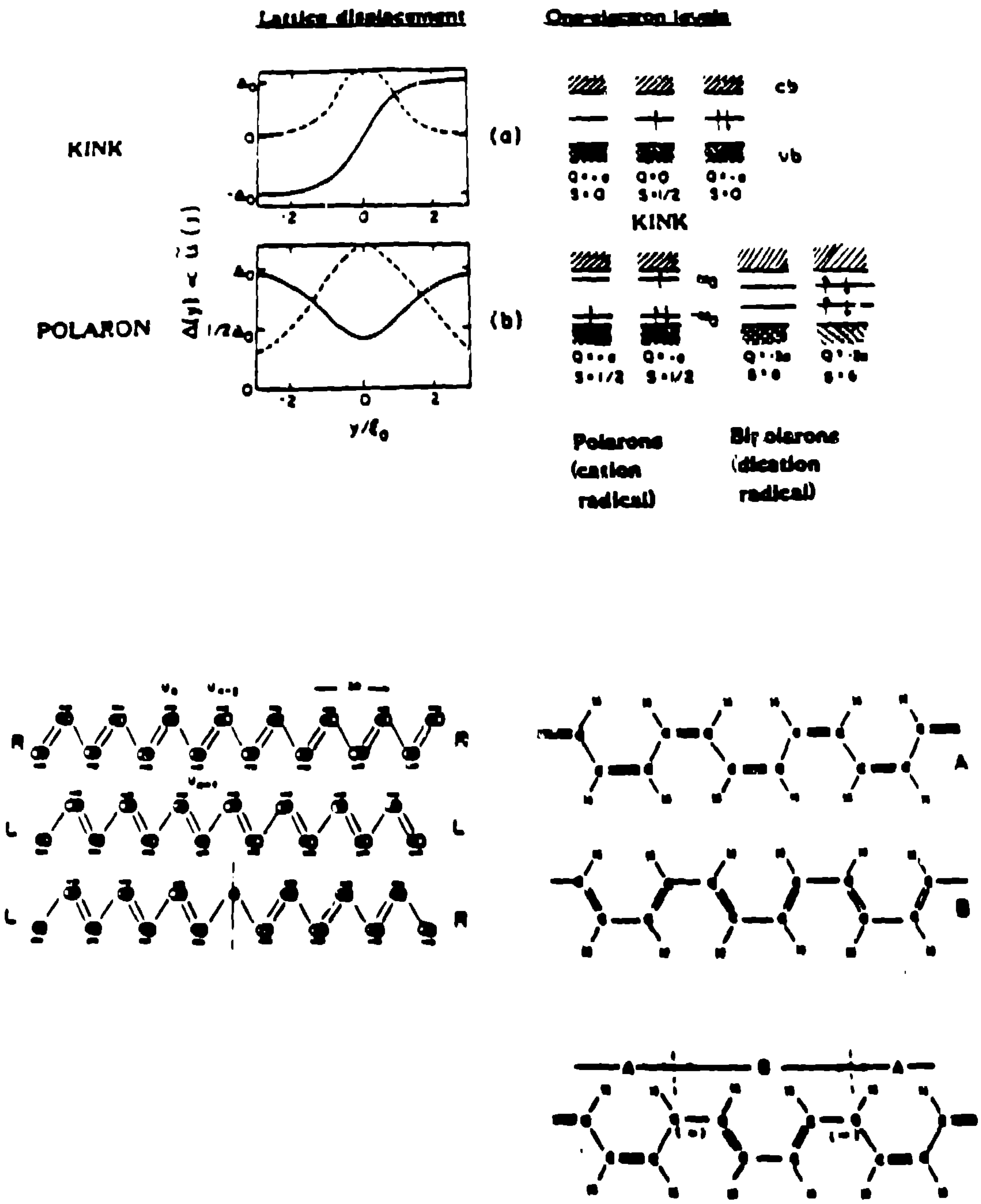


Figure 6. Lattice deformations and electronic levels corresponding to polarons and bipolarons in cis- and trans-polyacetylene.

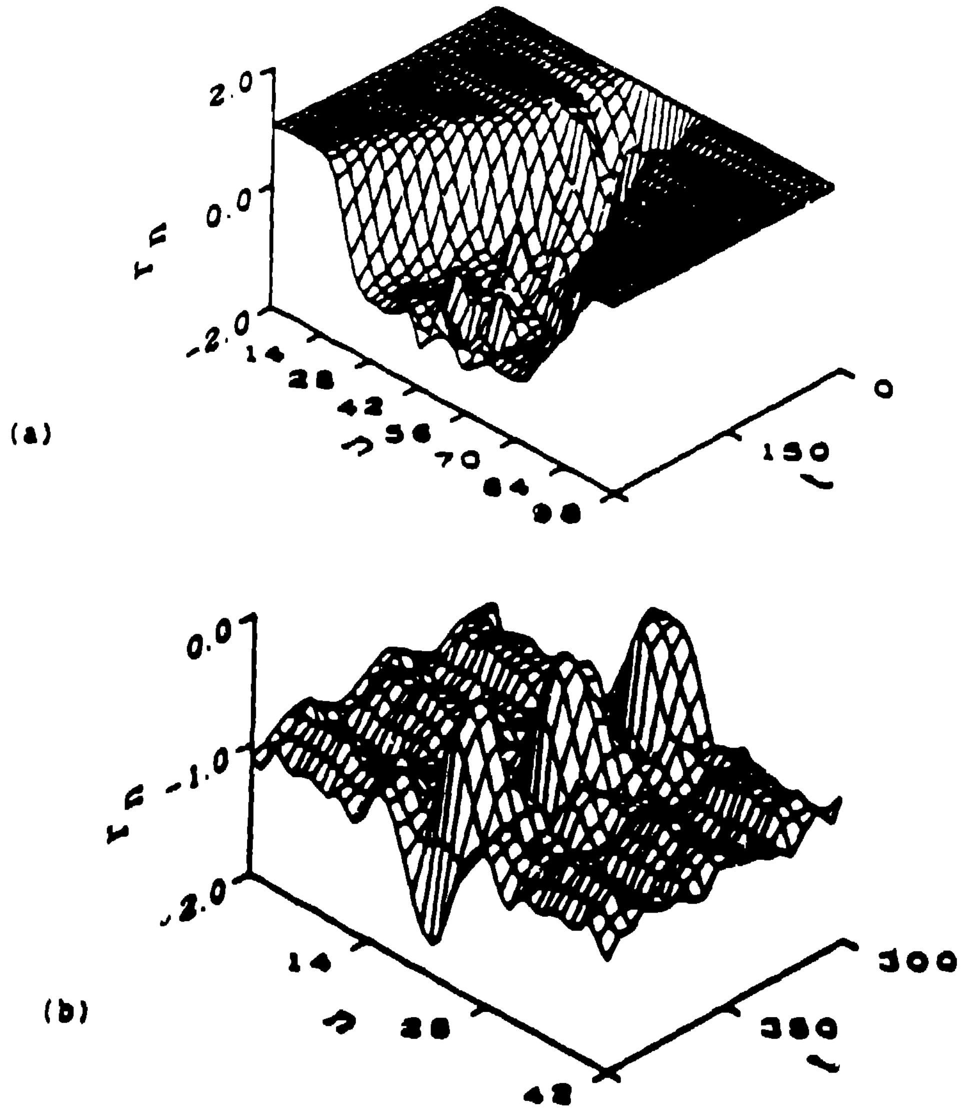


Figure 7. Breather formation following photoexcitation in a model of trans-polyacetylene.

where $\varepsilon$ is a small parameter. Semiclassical *quantization* of these breathers gives an energy spectrum [50]

$$E_B^Q = n\omega_R \left[1 - \frac{\pi^2}{72} \frac{\omega_R^2}{\Delta^2} n^2 + o(n^4)\right] \quad (n \; integer)$$

which shows that the breathers should be viewed as phonon bound states. The electron spectrum accompanying the breathing mode is dominated by two localized gap states (as in the polaron spectrum of Fig. 6) oscillating periodically to the gap edge and deeply into the gap [50]. They are expected to yield optical absorption signatures with absorption peaks near the band edge and associated bleaching of interband absorption, however this involves calculations beyond the adiabatic limit which are described in [51]. Picosecond resolved photo induced photoabsorption experiments [52] do indeed show such features but many decay channels are possible and have yet to be resolved (interchain excitons versus on-chain charge separation, "hot" solitons, $A_g$ correlation states, etc.).

Note that the electronic occupation of the breathing localized levels is neutral (lower level doubly occupied and upper level unoccupied). Chemically, this is a "zwitterion" intermediate species. Similar "breathing modes" (with various electronic occupations) have now been found to be extremely typical in this class of models -- examples include cis-polyacetylene, A-B polymers, polyyne chains, as well as photoexcitation in the presence of polarons and extrinsic impurities. They are essentially always a consequence of the anharmonic lattice dynamics resulting from electron-phonon coupling.

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